Stroboscopic quantization of autonomous systems

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Abstract

We introduce a semiclassical quantization method which is based on a stroboscopic description of the classical and the quantum flows. We show that this approach emerges naturally when one is interested in extracting the energy spectrum within a prescribed and *finite* energy interval. The resulting semiclassical expression involves a finite number of periodic orbits whose energies are in the considered interval. Higher order corrections which reflect the sharp restriction of the spectrum to an interval are explicitly given. The relation to Fourier methods for extracting semiclassical spectra, such as harmonic inversion, is worked out. The constraints due to the finite dimension of the Hilbert space and the unitarity of the restricted quantum evolution operator are important ingredients in this context.

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I. INTRODUCTION

The pioneering semiclassical quantization schemes introduced by Gutzwiller [1,2] (general chaotic hamiltonian flows) and Balian and Bloch (billiards) [3] are afflicted by a severe and intrisic problem: the semiclassical trace formulae and the spectral determinants derived from them involve an unlimited number of periodic orbits and do not converge on the real energy axis. Several authors proposed various solutions to this problem:

The cycle expansion [4–6] exploits the presence of correlations between long and short orbits to argue that a suitable rearrangement of the spectral determinant converges on the real axis. The improved convergence has been demonstrated for certain open systems like scattering off three disks [6,7] and for a map, the quantum bakers map [8]. Applications to bounded systems are typically troubled by the lack of a convenient symbolic coding and the presence of marginally stable periodic orbits that spoil the ideal exponential convergence [9,10].

Keating and Berry [11–13] made use of the analytic properties of the exact spectral determinant, and enforced it on the semiclassical expression, thus deriving a quantization scheme which is similar to the Riemann-Siegel formula for the Riemann ζ function on the critical line. Its main term involves a finite number of periodic orbits, and the further corrections are given explicitly and they are small in the semiclassical limit.

There are, however, alternative semiclassical quantization schemes for chaotic systems: One considers the quantum analogue of the classical evolution operator on a Poincaré surface of section of a finite volume [14–16]. The area preserving Poincaré map when quantized yields a semiclassically unitary evolution operator which acts on a Hilbert space of dimension $L = \begin{bmatrix} \frac{\mathcal{V}}{\hbar^f} \end{bmatrix}$, where \mathcal{V} is the phase space volume of the 2f dimensional section, and $[\cdot]$ stands for the integer part. Denoting by $S(E,\hbar)$ the $L\times L$ (semiclassically) unitary evolution operator, one expresses the quantization condition in terms of the secular function:

$$Z_{scl}(E;\hbar) = \det\left(I - S(E,\hbar)\right) , \qquad (1.1)$$

and the spectrum $\{E_n\}$ satisfies the quantization condition

$$Z_{scl}(E_n; \hbar) = 0. (1.2)$$

The secular function is nothing but the characteristic polynomial of S, $\det(I - zS(E, \hbar)) = \sum_{l=0}^{L} a_l(E, \hbar) z^l$ computed at z=1. The special symmetry of the Riemann-Siegel expression, which is a consequence of the functional equation in the Riemann- ζ function case, follows here from the unitarity of S. It implies the inversive identities

$$a_l = e^{i\Theta} a_{L-l}^* , (1.3)$$

where Θ stands for the phase of det $(-S(E,\hbar))$. When the semiclassical approximation is used to compute $Z_{scl}(E;\hbar)$, the coefficients a_l are expressed in terms of periodic orbits of the Poincaré map with periods up to l. Thus, the computation of the semiclassical secular equation requires only a finite number of periodic orbits.

This proceedure was used e.g. by Bogomolny [14] who derived a semiclassical approximation for the restriction of the Green function to the Poincaré section, and by Doron and Smilansky [15] who used the scattering approach, and identified the scattering matrix

as the unitary operator in equation (1.1). Further work along this line was carried out by Gutzwiller [17], Prosen [18] and others (for a review see e.g., [16]).

The reduction of the classical dynamics to a discrete, area preserving mapping, can also be achieved by observing the flow at fixed time intervals. It is our aim here to suggest a new quantization scheme which is based on the quantum mechanical analogue of the stroboscopic classical map. The resulting quantization scheme, which is developed in section (II), addresses the spectrum in a finite spectral interval of a size which is dictated by the dynamical system and by Planck's constant. It is similar in its formal structure to the methods which were briefly summerized above. However, it is based on the classical periodic orbits of a different map, and it offers both the leading and the next to leading order contributions in the semiclassical expression for the secular equation. The semiclassical version of the stroboscopic quantization is given in (II). Among the other consequences of our derivation we note a relation between the time steps in the evolution operator and the mean density of states, a consistent truncation of the periodic orbit series as well as conditions for self-inversiveness of the characteristic polynominal.

The idea of extracting eigenvalues within a certain energy band has many connections to frequently employed numerical schemes that also obtain eigenvalues within a certain frequency band. For instance, from the overlap of a wave packet with its propagated image over some time interval one can extract eigenvalues in a band near the initial energy [19]. The semiclassical procedure described here achieves the same without a weighting by the projection of initial wave packet onto eigenstates and moreover suggests a semiclassical approximation. A numerically accurate and efficient way of implementing this Fourier analysis has been developed by Neuheuser and Wall [20,21] and Mandelshtam and Taylor [22–24] in the form of harmonic analysis. The way harmonic analysis beats the resolution limit set by the Nyquist theorem is by implementing additional information on the Fourier signal. In the case of the traces it uses explicitly that they are sums of exponentials with a discrete set of frequencies. We will relate the basic ideas of harmonic analysis to the semiclassical traces and discuss the relation to the cycle expansion. The relation of the present formalism and harmonic inversion will be discussed in section (IV). A few concluding remarks and a summary will be the contents of section (V).

II. STROBOSCOPIC QUANTIZATION

We would like to compute a *finite* sequence of energy eigenvalues in the spectrum of an autonomous (time independent) quantum Hamiltonian H. This sequence is located in an energy interval \mathcal{E} ,

$$\mathcal{E} \equiv [E_0 - \Delta/2 , E_0 + \Delta/2].$$
 (2.1)

The midpoint of the interval E_0 is arbitrary, and its length Δ is $\approx \mathcal{O}(\hbar^{\gamma})$ where $1 > \gamma > 0$. This makes Δ small on the classical scale but large on the quantum scale since for a system with f degrees of freedom the mean spectral density $\bar{d}(E_0) \approx \mathcal{O}(\hbar^f)$. Hence the number of eigenenergies in the interval

$$N = \bar{d}(E_0) \ \Delta \,, \tag{2.2}$$

is large. Moreover, Δ is also sufficiently small so that $\bar{d}(E)$ is effectively constant in the interval.

Consider now the N dimensional Hilbert space spanned by the eigenvectors of H with eigenenergies in \mathcal{E} . The quantum evolution operator in this subspace can be projected from the full evolution operator $U(t) = e^{-iHt/\hbar}$. It is given explicitly by

$$\mathcal{U}(t;\mathcal{E}) = \sum_{E_n \in \mathcal{E}} |\psi_n\rangle e^{-iE_n t/\hbar} \langle \psi_n|$$
(2.3)

and

$$\operatorname{tr} \mathcal{U}(t; \mathcal{E}) = \sum_{E_n \in \mathcal{E}} e^{-iE_n t/\hbar} = \int \chi(E) \ d(E) e^{-iEt/\hbar} dE,$$
 (2.4)

where $\chi(E)$ is the characteristic function of \mathcal{E} , and

$$d(E) = \sum_{\nu=1}^{\infty} \delta(E - E_{\nu}) \tag{2.5}$$

is the density of states for the full system. We will use small greek indices to run over all eigenstates of the Hamiltonian and small latin ones if they are restricted to the energy interval \mathcal{E} .

Choose an as yet arbitrary time interval of length τ so that $\tau \Delta \leq 2\pi \hbar$. The N eigenvalues $e^{-iE_n\tau/\hbar}$ of the unitary matrix $\mathcal{U}(\tau;\mathcal{E})$ occupy an arc of the unit circle whose length is at most 2π , and therefore they preserve the order of the spectral sequence on \mathcal{E} . The spectrum of H in the interval \mathcal{E} can be identified as the zeros of the secular equation:

$$\zeta_{\mathcal{E}}(E) = \det\left(I - e^{\frac{i}{\hbar}E\tau} \mathcal{U}(\tau; \mathcal{E})\right). \tag{2.6}$$

In other words, whenever the eigenphases of $e^{\frac{i}{\hbar}E\tau} \mathcal{U}(\tau;\mathcal{E})$ take the value 1, a spectral point of H is encountered. Because of the exponentiation and the restriction to a finite set of eigenenergies in the interval \mathcal{E} , the density of states derived from this secular equation is a train of delta functions at the positions of the eigenenergies E_n , periodically continued by a separation $\hbar/2\pi\tau$,

$$d(E; \mathcal{E}) = \tau/\hbar \sum_{m=-\infty}^{\infty} \sum_{n:\{E_n \in \mathcal{E}\}} \delta(\tau(E - E_n)/\hbar + 2\pi m)$$

$$= \frac{N\tau}{2\pi\hbar} + \frac{\tau}{2\pi\hbar} \sum_{m=1}^{\infty} \left\{ e^{-imE\tau/\hbar} \operatorname{tr} \mathcal{U}^m(\tau; \mathcal{E}) + c.c. \right\}$$

$$= \frac{N\tau}{2\pi\hbar} + \frac{\tau}{2\pi\hbar} \sum_{m=1}^{\infty} \left\{ e^{-imE\tau/\hbar} \operatorname{tr} \mathcal{U}(m\tau; \mathcal{E}) + c.c. \right\}.$$

The second line follows from Poisson summation of the first line. As usual, the density of states can be split into a smooth part and an oscillatory part, where the latter should vanish when averaged over the energy interval $\hbar/2\pi\tau$. In the semiclassical limit, the traces $\operatorname{tr} \mathcal{U}^m(\tau;\mathcal{E})$ are expressed as sums over periodic orbits, which give the oscillatory part of the spectral density. The smooth parts of both sides of (2.7) must be identical, which defines τ uniquely as

$$\tau = \frac{2\pi\hbar\bar{d}(E_0)}{N} = \frac{\tau_H}{N}, \qquad (2.7)$$

where τ_H is the Heisenberg time.

This choice of the value of τ completely determines the quantum map $\mathcal{U}(\tau; \mathcal{E})$ which provides us through (2.7) with the spectral density of H in \mathcal{E} . This is a *stroboscopic* map, since τ is fixed. The unitarity of $\mathcal{U}(\tau; \mathcal{E})$ is an important asset, since one can write the secular equation in a form which exploits naturally the inversive symmetry of the coefficients of the characteristic polynomial of $\mathcal{U}(\tau; \mathcal{E})$. Writing

$$\zeta_{\mathcal{E}}(E) = \det\left(I - e^{iE\tau/\hbar} \mathcal{U}(\tau; \mathcal{E})\right) = \sum_{n=0}^{N} a_n e^{inE\tau/\hbar},$$
(2.8)

the inversive symmetry is expressed by the identity

$$a_n = e^{i\Theta} a_{N-n}^* , (2.9)$$

where Θ stands for the phase of $\det(-\mathcal{U}(\tau;\mathcal{E}))$. We use

$$\det\left(-e^{iE\tau/\hbar} \ \mathcal{U}(\tau;\mathcal{E})\right) = e^{-i\pi N + i2\pi(E - E_0)\bar{d}(E_0)} = e^{i2\pi\bar{N}(E,E_0)} , \qquad (2.10)$$

where we introduced the smooth spectral counting function in the energy interval \mathcal{E} , $\bar{N}(E, E_0) = (E - E_0)\bar{d}(E_0) - N/2$. Thus,

$$e^{i\pi \ \bar{N}(E,E_0)}\zeta \ \varepsilon(E) = \sum_{n=0}^{[N/2]} \left\{ a_n e^{i\pi \ \bar{N}(E,E_0)} + a_n^* e^{-i\pi \ \bar{N}(E,E_0)} \right\} + \epsilon_N a_{N/2} e^{i\pi \ \bar{N}(E,E_0)} \ . \tag{2.11}$$

As before, [x] stands for the largest integer smaller than x, and $\epsilon_N = 1$ if N is even and $\epsilon_N = 0$ otherwise.

The cycle expansion [26–28] and Newton's identities relate the traces $t_n = \operatorname{tr} \mathcal{U}^n(\tau; \mathcal{E})$ and the coefficients of the characteristic polynomial

$$a_n = -\frac{1}{n} \left(t_n + \sum_{k=1}^{n-1} a_k t_{n-k} \right) . {(2.12)}$$

The inversive symmetry halves the number of coefficients needed to calculate the spectral secular equation. This symmetry is a consequence of the unitarity of the evolution operator and as such it is the expression of a basic property of the quantum evolution - the conservation of probability (norm). The semiclassical theory provides approximate expressions to t_n which are used to compute the a_n using Newton's identities. The resulting semiclassical secular function is similar in many ways to the expressions derived by Berry and Keating [11–13], Bogomolny [14], and Doron and Smilansky [15,16]. It will be discussed in the sequel.

III. THE SEMICLASSICAL APPROXIMATION

It is convenient to introduce the semiclassical approximation by writing (2.4) as

$$\operatorname{tr} \mathcal{U}(t; \mathcal{E}) = \int \chi(E) d(E) e^{-iEt/\hbar} dE$$

$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} ds \ \hat{\chi}(s) \ \operatorname{tr} U(t+s) , \qquad (3.1)$$

where

$$\hat{\chi}(s) = \int_{-\infty}^{\infty} \chi(E) e^{\frac{i}{\hbar} E s} dE = e^{iE_0 s/\hbar} \frac{\sin \frac{s\Delta}{2\hbar}}{\frac{s}{2\hbar}}, \qquad (3.2)$$

and where $U(t) = e^{-iHt/\hbar}$ is the evolution operator of the *entire* system. We can then use the semiclassical expression for $\operatorname{tr} U(t)$ for any time t, given by

$$[\operatorname{tr} U(t)]_{scl} = \frac{t}{(2\pi i\hbar)^{1/2}} \sum_{p \in \mathcal{P}(t)} \left(\frac{\mathrm{d}E_p}{\mathrm{d}t}\right)^{1/2} \frac{\mathrm{e}^{iR_p/\hbar - i\nu_p\pi/2}}{\left|\det(I - M_p)\right|^{1/2}}, \tag{3.3}$$

where $\mathcal{P}(t)$ is the set of t-periodic orbits and

$$R_p = \int_0^t [p_p(t)\dot{q}_p(t) - H(q_p(t), p_p(t))] dt.$$
 (3.4)

The building blocks for the semiclassical theory are the traces $\operatorname{tr} \mathcal{U}^n(\tau; \mathcal{E})$. By an exact quantum identity they coincide with $\operatorname{tr} \mathcal{U}(n\tau; \mathcal{E})$, so that we need to compute the traces for times which are integer multiples of τ . Notice that the periodic orbits $p \in \mathcal{P}(t)$ which contribute to (3.3) can have arbitrary energies $E_p(t)$. They are functions of the period $t = n\tau$ which is fixed. Substituting (3.3) in (3.1),

$$[\operatorname{tr} \mathcal{U}(n\tau;\mathcal{E})]_{scl} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \mathrm{d}s \,\,\hat{\chi}(s) \,\, [\operatorname{tr} U(n\tau+s)]_{scl}$$

$$\approx \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \mathrm{d}s \,\,\hat{\chi}(s) \,\, \frac{n\tau+s}{(2\pi i\hbar)^{1/2}} \,\, \sum_{p \in \mathcal{P}(n\tau+s)} \left(\frac{\mathrm{d}E_p}{\mathrm{d}t}\right)^{1/2} \frac{\mathrm{e}^{iR_p/\hbar - i\nu_p\pi/2}}{\left|\det(I-M_p)\right|^{1/2}} \,. \quad (3.5)$$

The range of $\hat{\chi}(s)$ is determined by the time $\frac{\hbar}{\Delta} \approx \mathcal{O}(\hbar^{1-\gamma})$ which is classically short. Hence we can approximate the integral over the periodic orbit sum by expanding the phase of the integrand about t. For this purpose we use $\frac{\partial R_p(t)}{\partial t} = -E_p(t)$. Denoting the preexponential amplitudes in (3.5) by $A_p(t)$, we use $A_p(n\tau + s) \approx A_p(n\tau)$ which is consistent with the semiclassical approximation. The contribution of each periodic orbit will be

$$\frac{A_{p}(n\tau)}{2\pi\hbar} e^{\frac{i}{\hbar}S_{p}(n\tau)} \int_{-\infty}^{\infty} ds \, \frac{\sin\frac{s\Delta}{2\hbar}}{\frac{s}{2\hbar}} e^{\frac{i}{\hbar}\left[(E_{0}-E_{p}(t))s-\frac{1}{2}\frac{dE_{p}}{dt}s^{2}\right]}$$

$$= A_{p}(n\tau) e^{\frac{i}{\hbar}S_{p}(n\tau)} \left(\frac{-i}{2}\right)^{\frac{1}{2}} \left\{ \left[C(x_{p}^{+}(n\tau)) + iS(x_{p}^{+}(n\tau))\right] - \left[C(x_{p}^{-}(n\tau)) + iS(x_{p}^{-}(n\tau))\right] \right\} , \quad (3.6)$$

where C and S are the cos and sin Fresnel integrals with the argument

$$x_p^{\pm}(n\tau) = \frac{E_p(n\tau) - E_0 \pm \frac{\Delta}{2}}{\left(2\hbar \left|\frac{\mathrm{d}E_p}{\mathrm{d}t}\right|\right)^{\frac{1}{2}}}$$
(3.7)

In the above expression, the difference of the energy of the periodic orbit, $E_p(n\tau)$, from the interval of interest \mathcal{E} , is measured in units of the energy scale $(2\hbar \left| \frac{\mathrm{d}E_p}{\mathrm{d}t} \right|)^{\frac{1}{2}}$. (we assumed throughout the derivation that, as is typically the case, $\frac{\mathrm{d}E_p}{\mathrm{d}t}$ is negative.) Using dimensional analysis one can bound this scale from above by $\mathcal{O}\left(\hbar^{\frac{1-\gamma}{2}}\right)$, which is small on the classical scale. Using the asymptotic expression for the Fresnel integral for large argument,

$$C(x) + iS(x) \approx \left(\frac{i}{2}\right)^{\frac{1}{2}} \operatorname{sign}(x) - \frac{i}{x\pi} e^{i\frac{\pi}{2}x^2} + \mathcal{O}\left(\frac{1}{|x|^3}\right). \tag{3.8}$$

The difference between the Fresnel integrals in (3.6) is dominated in the semiclassical limit by the contribution of the leading term in (3.8) which, together with the factor $(-i/2)^{1/2}$ (see (3.6)) is the characteristic function of the spectral interval \mathcal{E} . Thus, the leading semiclassical contribution makes use of periodic orbits whose energy $E_p(t)$ is in \mathcal{E} and does not take into account the "diffractive" effects due to the sharp restriction of the spectrum to the interval \mathcal{E} . The Fresnel functions with finite arguments include the appropriate corrections.

The semiclassical approximation for the $[t_n]_{scl} = [\operatorname{tr} \mathcal{U}(n\tau;\mathcal{E})]_{scl}$ is obtained by summing the amplitudes (3.6) over the set $\mathcal{P}(n\tau)$ of periodic orbits. When $[t_n]_{scl}$ is substituted in (2.11) one obtains the semiclassical spectral secular equation. It can be written as a sum of two parts. The first is obtained from the leading semiclassical expression for t_n . It uses the periodic classical orbits of period $n\tau$ with energies in the interval of interest \mathcal{E} . The diffractive corrections go beyond this limit, and apart from modifying the contributions of "allowed" periodic orbits, it introduce the effects of periodic orbits whose energies are outside the strict energy interval. These corrections are analogous to the expressions derived by Berry and Keating [11–13] which are missing in the derivations based on the Poincaré section [14] or the scattering approaches to quantization [15,16]. Here, one can attribute them to the sharp truncation of the energy domain and their main effect is the inclusion of evanescent, classically forbidden contributions.

Finally, we would like to mention that the semiclassical approximation could be introduced in a different way. With

$$P(\mathcal{E}) = \sum_{n:\{E_n \in \mathcal{E}\}} |n\rangle\langle n|, \qquad (3.9)$$

the projector onto the energy interval, we have the quantum identity

$$\operatorname{tr} \mathcal{U}^{n}(\tau; \mathcal{E}) = \operatorname{tr} \mathcal{U}(n\tau; \mathcal{E}) = \operatorname{tr} \left(P(\mathcal{E})U(\tau)\right)^{n}.$$
 (3.10)

The semiclassical approximation we used in (3.3) and (3.5) is

$$\operatorname{tr} \mathcal{U}^{n}(\tau) \sim \left[\operatorname{tr} \mathcal{U}(n\tau)\right]_{scl}$$
 (3.11)

The alternative approximation

$$\operatorname{tr} \mathcal{U}^{n}(\tau) \sim \operatorname{tr} \left([P(\mathcal{E})U(\tau)]_{scl} \right)^{n} .$$
 (3.12)

would contain a product of Fresnel factors that reduces to (3.5) only to leading order. Such differences are not uncommon in attempts to go beyond the leading order in the semiclassical approximation. We favor the representation (3.11) since it makes use of as much exact quantum information as possible and leaves the semiclassical approximation only to the very end.

IV. OBTAINING EIGENVALUES

Given the traces of $\mathcal{U}(n\tau)$ at equidistant time intervals τ , the extraction of eigenvalues becomes a problem in Fourier inversion. If all traces tr \mathcal{U}^m in (2.7) and (2.12) are known, the relation is exact. However, in practice only a finite number of traces can be calculated, and then standard Fourier inversion is limited in resolution by the Nyquist sampling theorem, which for traces up to N implies a resolution of the order of the mean spacing. Additional errors are introduced by the semiclassical approximation. In order to go beyond the limit of resolution set by the Nyquist theorem additional information has to be added to the Fourier inversion. For the case at hand, harmonic inversion [20–25] is particularly appropriate. It assumes that the signal is composed of a finite number of frequencies and provides an efficient method for solving the ensuing approximation problem. Specifically, it uses the traces to set up a matrix V that has the same eigenvalues as \mathcal{U} , so that the frequencies can be found from the traces by an eigenvalue determination, which numerically is more reliable than a standard search for zeroes. Note that the matrix V has the same eigenvalues as \mathcal{U} , but it will usually not be unitary. In the description of harmonic analysis below we will emphasise the matrix structure and its origin and will omit numerical issues such as windowing and the like.

Let N be the fixed dimension of the matrix \mathcal{U} and let, as before,

$$t_m = \operatorname{tr} \mathcal{U}^m = \sum_{n=1}^N e^{-im\phi_n}, \qquad (4.1)$$

be the traces of the m-th power of the unitary operator. In the quantum case the phases $\phi_n = E_n \tau / \hbar$ are real and contain the eigenenergies. In the semiclassical approximation they may become complex, in which case the imaginary parts can be used as a measure of the semiclassical error. The form (4.1) of the traces implies that t_n for n > N can be expressed as a linear combination of the traces t_m with indices m < N, as in the case of autoregressive models. Harmonic inversion exploits these relations for the construction of a matrix \tilde{V} that has the same eigenvalues as \mathcal{U} . To derive this matrix, define an N-dimensional vector \mathbf{t}_m of traces starting with t_m , i.e.,

$$\mathbf{t}_m = \begin{pmatrix} t_m \\ \vdots \\ t_{m+N-1} \end{pmatrix}, \tag{4.2}$$

the N-dimensional vector $\mathbf{I} = (1, \cdots, 1)^T$ and the auxiliary $N \times N$ matrix

$$\Omega_{m,n} = e^{-im\phi_n} \,. \tag{4.3}$$

Then

$$\mathbf{t}_1 = \Omega \mathbf{I} \,. \tag{4.4}$$

For higher m the vectors \mathbf{t}_m can be represented as

$$\mathbf{t}_m = \Omega V^{m-1} \mathbf{I} \,. \tag{4.5}$$

with the diagonal matrix

$$V_{m,n} = e^{-i\phi_n} \delta_{m,n} \,. \tag{4.6}$$

The aim is to find a matrix \tilde{V} that is similar to V, so that the frequencies can be determined from the eigenvalues of \tilde{V} . To this end solve (4.4) for **I** and substitute in (4.5):

$$\mathbf{t}_m = \Omega V^{m-1} \Omega^{-1} \mathbf{t}_1 \,. \tag{4.7}$$

Since also

$$\mathbf{t}_{m+k} = \Omega V^{m-1} V^k \Omega^{-1} \mathbf{t}_1 = \left(\Omega V^{m-1} \Omega^{-1} \right) \left(\Omega V^k \Omega^{-1} \mathbf{t}_1 \right)$$
$$= \Omega V^{m-1} \Omega^{-1} \mathbf{t}_{k+1} , \tag{4.8}$$

it is possible to construct the full matrix

$$\tilde{V}_{m-1} = \Omega V^{m-1} \Omega^{-1} \tag{4.9}$$

from the images of the vectors \mathbf{t}_n for different n. Specifically, for m=2, the entries for the first iterate of \tilde{V} are

$$\mathbf{t}_{k+2} = \tilde{V}_1 \mathbf{t}_{k+1} \,. \tag{4.10}$$

This result shows that the matrix \tilde{V}_1 can be constructed from the traces (assuming that the eigenvalues are not identical and the vectors of traces not linearly dependent). The matrix \tilde{V}_1 is neither unitary nor symmetric but nevertheless has the eigenvalues $\exp(-i\phi_n)$.

It is possible to proceed one step further and to derive the characteristic polynominal. With the $N \times N$ matrices

$$T_{M} = \begin{pmatrix} t_{M} & t_{M-1} & \cdots & t_{M-N+1} \\ t_{M+1} & t_{M} & \cdots & t_{M-N+2} \\ \vdots & \vdots & & \vdots \\ t_{M+N-1} & t_{M+N-2} & \cdots & t_{M} \end{pmatrix}, \tag{4.11}$$

the relation (4.10) becomes

$$T_{N+1} = \tilde{V}_1 T_N \,, \tag{4.12}$$

so that formally $\tilde{V}_1 = T_N(T_{N+1})^{-1}$. Since N-1 columns in T_{N+1} and T_N coincide (up to a shift to the right), \tilde{V}_1 has the form

$$\tilde{V}_{1} = \begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & & \vdots \\
b_{N} & b_{N-1} & b_{N-2} & b_{N-3} & \cdots & b_{1}
\end{pmatrix},$$
(4.13)

where the vector $\mathbf{b} = (b_N, b_{N-1}, \dots, b_1)$ solves

$$\begin{pmatrix} t_{2N-1} \\ t_{2N-2} \\ \vdots \\ t_{N-1} \end{pmatrix} = T_N^T \begin{pmatrix} a_N \\ a_{N-1} \\ \vdots \\ a_1 \end{pmatrix}. \tag{4.14}$$

Exploiting this special form of the matrix \tilde{V}_1 and the vector **b** the Fredholm determinant can be expanded

$$F(z) = \det(1 - z\tilde{V}_1) = 1 - \sum_{k=1}^{N} z^k b_k.$$
(4.15)

Since the eigenvalues of \mathcal{U} and \tilde{V}_1 are the same, the coefficients of the characteristic polynominals (2.8) and (4.15) also have to be the same, up to an overall scale factor.

It is important to note one significant difference, though: in the derivation of the polynominal for the quantum operator \mathcal{U} , traces up to order N determined all coefficients and self inversivness allowed to bring this number down to N/2. In the harmonic inversion case the number of traces needed is 2N+1. The origin of this difference is the fact that in the case of the harmonic inversion nothing changes in the formalism if the traces $\mathrm{tr}\mathcal{U}^n$ are replaced by $\mathrm{tr}\mathcal{A}\mathcal{U}^n$ with some operator A: the set up for the matrix \tilde{V}_1 remains the same, but the coefficients of the vector \mathbf{I} change. If A=1, then traces with n>N can be expressed by traces of lower order using Cayley's theorem. Thus, harmonic inversion is more general in its basic structure, but also more wasteful in the number of traces required. In addition, it is difficult to see how properties such as self-inversiveness can be implemented directly (they can always be put in by hand in the characteristic polynominal).

V. CONCLUDING REMARKS

The main features of stroboscopic quantization are the limitation to a finite interval in energy, the semiclassical expression with a finite number of periodic orbits and the finite characteristic polynominal. The origin of the finite representation is a physical one, the limitation to a finite interval in energy. Other modifications of the Gutzwiller trace formula, such as a Gaussian truncation or even a sharp cut-off, arrive at this restriction at the price of smearing the eigenvalues. Moreover, since with these smearings the evolution operator is not confined to a finite interval, the characteristic function is not a polynominal anymore and the conditions of self-inversiveness are difficult to implement.

The weight of periodic orbits and in particular the Fresnel corrections bear a striking similarity to the error function truncations introduced by Berry and Keating on the level of the Fredholm product [11–13]. Note, however, that the product of two Fresnel integrals is not a Fresnel integral of the sum of the arguments, so that the modification that would apply to a pseudo-orbit differs from the product of the weights of the original orbits.

On the numerical side, the results on stroboscopic quantization suggest that for harmonic analysis the time period τ over which the evolution operator is followed should be fixed to be τ_H/N , so that an optimal characteristic polynominal that shows self-inversiveness results. Ideally, one would like to improve the method so as to use only the linearly independent N/2 traces, but it is not clear how that can be implemented other than by brute force.

The finiteness of the characteristic polynominal results from the quantum fact that after the projection onto the energy interval the Hilbert space is finite dimensional and that there are only a finite number of eigenvalues. In particular, this implies relations between traces of higher powers of \mathcal{U} due to Cayley's theorem. Within the semiclassical approximation no such constraint and no such relation between traces of higher and lower powers are evident. In many approaches [11–16] they are put in by hand and justified by appeal to the properties of the quantum propagator. However, it is legitimate to ask to which extend the semiclassical approximation reflects these properties by itself, and it is comforting to note that, as demonstrated for the Bakers map [8] and also for the three disk scattering system [6,7,30], where none of these unitarity arguments apply, the coefficients in the cycle expansion beyond the dimension of the system decay.

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REFERENCES

- [1] M. C. Gutzwiller, Chaos in Classical and Quantum Mechanics, Springer (New York 1990).
- [2] M. C. Gutzwiller, J. Math. Phys. 8, 1979 (1967); J. Math. Phys. 10, 1004 (1969); J. Math. Phys. 11, 1791 (1970)
- [3] C. Bloch and R. Balian, Ann. Phys. 69, 76 (1972).
- [4] P. Cvitanović, and B. Eckhardt, Phys. Rev. Lett. **63**, 823 (1989)
- [5] B. Eckhardt, Proceedings of the International School of Physics "Enrico Fermi", Course CXIX "Quantum Chaos", G. Casati, I. Guarneri, and U. Smilansky (eds), North Holland, Amsterdam, 1993, p. 77.
- [6] B. Eckhardt, G. Russberg, P. Cvitanović, P.E. Rosenqvist and P. Scherer, in *Quantum Chaos*, G. Casati, B. V. Chirikov (eds), Cambridge University Press, p. 405.
- [7] A. Wirzba, Phys. Rep. **309**, 2 (1999) .
- [8] B. Eckhardt and F. Haake, J. Phys A: Math. Gen. 27, 4449 (1994).
- [9] G. Tanner, Nonlinearity **9**, 1641 (1996).
- [10] P. Dahlvist, Chaos, Solitons and Fractals, 8, 1011 (1997) .
- [11] M.V. Berry and J. Keating, J. Phys. A: Math. Gen. 23 4839 (1990).
- [12] M.V. Berry and J.P. Keating, *Proc. R. Soc. (London)* **437**, 151 (1992) .
- [13] J.P. Keating, Proc. R. Soc. (London) 436, 99 (1992) .
- [14] E.B. Bogomolny, *Nonlinearity* 5, 805 (1992).
- [15] E. Doron and U. Smilansky. *Nonlinearity* **5** 1055, (1992).
- [16] U. Smilansky, in *Proc. of the Les Houches Summer School on Mesoscopic Quantum Physics*. Elsevier Science Publ. (1995) Ed. E. Akkermans, G. Montambaux and J. L. Pichard.
- [17] M. C. Gutzwiller, Chaos 3, 591 (1993).
- [18] T. Prosen, J. Phys. A 28, 4133 (1995); Physica D 91, 244 (1995) .
- [19] E.J. Heller, in *Proc. of the Les Houches Summer School on Chaos and Quantum Physics*, Ed. M. J. Giannoni, A. Voros and J. Zinn-Justin (eds)., North Holland (1989), p. 547.
- [20] D. Neuhauser, J. Chem. Phys. 93, 2611 (1990).
- [21] M. R. Wall and D. Neuhauser, J. Chem. Phys. $\mathbf{102},\,8011$ $(1995)\,.$
- [22] V. A. Mandelshtam and H. S. Taylor, Phys. Rev. Lett. ${\bf 78},\,3274$ $(1997)\,.$
- [23] V. A. Mandelshtam and H. S. Taylor, J. Chem. Phys. **107**, 6756 (1997).
- $[24]~{\rm V.~A.~Mandelshtam,~J.~Chem.~Phys.~\bf 108,~9999~(1998)}\,.$
- [25] J. Main, Phys. Rep. **316**, 234 (1999).
- [26] J. Plemelj, Monat. Math. Phys. **15**, 93 (1909).
- [27] F. Smithies, Duke Math. J. 8 $107\ (1941)\,.$
- [28] M. Reed and B. Simon, Methods of Modern Mathematical Physics vol 4 Analysis of Operators, Academic Press (New York 1978).
- [29] M.V. Berry and K.E. Mount, Rep. Prog. Phys. ${\bf 35},\,315$ (1972) .
- [30] B. Eckhardt and G. Russberg, Phys. Rev. E $\mathbf{47},\,1578$ (1993) .